

**REGULAR MULTIGRAPHS AND THEIR APPLICATION
TO THE MONTE CARLO EVALUATION OF MOMENTS
OF NON-LINEAR FUNCTIONS OF GAUSSIAN
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This paper expands on the multigraph method for expressing moments of non-linear functions of Gaussian random variables. In particular, it includes a list of regular multigraphs that is needed for the computation of some of these moments. The multigraph method is then used to evaluate numerically the moments of non-Gaussian self-similar processes. These self-similar processes are of interest in various applications and the numerical value of their marginal moments yield qualitative information about the behavior of the probability tails of their marginal distributions.

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|-------------|------------------------|
| Multigraph | self-similar processes |
| moments | Hermite polynomials |
| Monte Carlo | Hermite processes |
| hydrology | |

1. Introduction

Moments of non-linear functions of Gaussian random variables can be expressed in terms of the correlations of these Gaussian variables. They can also be obtained from the cumulants or semi-invariants [9]. When the non-linear functions are represented as a linear combination of Hermite polynomials or as Wiener-Itô integrals, the multigraph method of Taqqu [10] or the diagram method of Dobrushin [2] can be used for numerical calculations.

In this paper, we investigate the practical problems related to the implementation of the multigraph method. The method is used here to evaluate numerically the moments of the Hermite processes $\{\bar{Z}_m(t), -\infty < t < \infty\}$, $m = 1, 2, \dots$, defined below in (1.1). In many applications one possesses estimates of the marginal moments and one wishes to compare these with the theoretical moments of a potential model. One resorts to moments when the distribution of the potential models is not explicitly available. This is presently the case for $\bar{Z}_m(t)$ for all values

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of m greater than 1. The processes $\bar{Z}_m(t)$ are of interest in many fields. They are important in probability theory because of their connection to central limit theorems involving strongly dependent random variables. Their significance for physics lies in their relevance to the renormalization group theory. They can also be used in practical modelling of geophysical phenomena (see [3] and [7] for recent surveys).

One possible way of defining the Hermite processes $\bar{Z}_m(t)$ is by using a Wiener-Itô representation [6]:

$$\begin{aligned} \bar{Z}_m(t) = C(m, D) \int_{-\infty}^t dB(\xi_1) \int_{-\infty}^{\xi_1} dB(\xi_2) \cdots \int_{-\infty}^{\xi_{m-1}} dB(\xi_m) \\ \times \int_0^t \prod_{i=1}^m (s - \xi_i)^{-D/2-1/2} 1(\xi_i < s) ds. \end{aligned} \quad (1.1)$$

Here $B(\xi)$ is the standard Brownian motion, $1(\cdot)$ denotes an indicator function and D is a constant satisfying

$$0 < D < 1/m.$$

It is then easy to see that $\bar{Z}_m(t)$ is self-similar with parameter

$$H = 1 - \frac{1}{2}mD \in (\frac{1}{2}, 1),$$

that is, for all $a > 0$, the finite-dimensional distributions of $\bar{Z}_m(at)$ are the same as those of $a^H \bar{Z}_m(t)$. The normalization constant

$$C(m, D) = \left\{ \frac{m! (1 - mD)(2 - mD)(\Gamma(\frac{1}{2}(1 + D)))^m}{2(\Gamma(\frac{1}{2}(1 - D))\Gamma(D))^m} \right\}^{1/2}$$

ensures that $E \bar{Z}_m^2(1) = 1$. The process $\bar{Z}_m(t)$ then has zero mean, covariance

$$E \bar{Z}_m(s) \bar{Z}_m(t) = \frac{1}{2} \{|s|^{2H} + |t|^{2H} - |s - t|^{2H}\}, \quad (1.2)$$

and increments $\bar{Z}_m(t+1) - \bar{Z}_m(t)$ which exhibit a *long-range dependence*, that is, as $s \rightarrow \infty$,

$$E\{\bar{Z}_m(t+s+1) - \bar{Z}_m(t+s)\}\{\bar{Z}_m(t+1) - \bar{Z}_m(t)\} \sim H(2H-1)s^{2H-2}.$$

Obviously, the larger the value of H , the stronger the dependence.

Further technical details about $\bar{Z}_m(t)$ can be found in [12, 13, 3].

The representation (1.1) does not directly yield information about the finite-dimensional distributions of the Hermite processes. In fact, hardly anything is known about these distributions, with one obvious exception: when $m = 1$, the process is Gaussian and its finite-dimensional distributions are therefore multivariate normal with mean 0 and covariance (1.2).

However, when $m \geq 2$, one can obtain some qualitative information about the behavior of the probability tails by evaluating numerically the marginal moments of $\bar{Z}_m(t)$.

The numerical values of $E(\bar{Z}_m(1))^p$ for $p = 3$ up to 6, $m = 2, 3, \dots, 8$ and $H = 0.6, 0.7, 0.8, 0.9$ are listed in Table 4. The moments are increasing functions of both m and H for the above values of the parameters. This suggests that, for fixed t , the probability tails of $\bar{Z}_m(t)$ become fatter as m and H increase. This information is of particular importance in hydrology where significant deviations from the mean are often observed.

The listings of Tables 1 and 2 and Fig. 1 relate to the multigraph method. They shed some light on the structure of the relevant multigraphs and they can be used to simplify the numerical evaluation of the moments of other non-linear functions of Gaussian random variables.

2. Moments of $\bar{Z}_m(1)$

The moments of $\bar{Z}_m(1)$ have been derived in earlier papers [10, 11]. They are as follows:

$$E(\bar{Z}_m(1))^p = \begin{cases} 0 & \text{when } p = 1 \text{ or } mp \text{ is odd,} \\ K^p \frac{(m!)^p}{2^{n: p/2} (\frac{1}{2} mp)!} \sum R(i_1, j_1, i_2, j_2, \dots, i_q, j_q) & \text{when } p \geq 2 \text{ or } mp \text{ is even.} \end{cases} \quad (2.1)$$

In the preceding expression,

$$K = \left(\frac{(1-mD)(2-mD)}{2(m!)} \right)^{1/2}, \quad q = \frac{1}{2} mp,$$

$$R(i_1, j_1, i_2, j_2, \dots, i_q, j_q) =$$

$$= \int_0^1 \cdots \int_0^1 |x_{i_1} - x_{j_1}|^{-D} |x_{i_2} - x_{j_2}|^{-D} \cdots |x_{i_q} - x_{j_q}|^{-D} dx_1 \cdots dx_p,$$

and \sum is a sum over all indices $i_1, j_1, i_2, j_2, \dots, i_q, j_q$ satisfying

- (i) $i_1, j_1, i_2, j_2, \dots, i_q, j_q \in \{1, 2, \dots, p\}$,
- (ii) $i_1 \neq j_1, i_2 \neq j_2, \dots, i_q \neq j_q$,
- (iii) each number $1, 2, \dots, p$ appears exactly m times in $(i_1, j_1, i_2, j_2, \dots, i_q, j_q)$.

Remarks. (1) We shall henceforth suppose $p \geq 2$ or mp even. When these conditions are not met, the moments are identically zero.

(2) Because of the self-similarity, the relation

$$E(\bar{Z}_m(t))^p = t^{Hp} E(\bar{Z}_m(1))^p$$

holds for any fixed value of t . Consequently, all the marginal moments can be straightforwardly obtained from those evaluated at $t = 1$.

(3) The finite-dimensional moments $E \bar{Z}_m(t_1) \bar{Z}_m(t_2) \cdots \bar{Z}_m(t_p)$ satisfy the same expression as $E(\bar{Z}_m(1))^p$, but with $R(i_1, j_1, i_2, j_2, \dots, i_q, j_q)$ in the right-hand side of (2.1) replaced by

$$\begin{aligned} R_{(t_1, t_2, \dots, t_p)}(i_1, j_1, i_2, j_2, \dots, i_q, j_q) &= \\ &= \int_0^{t_1} \int_0^{t_2} \cdots \int_0^{t_p} |x_{i_1} - x_{j_1}|^{-D} |x_{i_2} - x_{j_2}|^{-D} \cdots |x_{i_q} - x_{j_q}|^{-D} dx_1 dx_2 \cdots dx_p. \end{aligned} \quad (2.2)$$

(4) Suppose that (X_1, X_2, \dots, X_p) is a multivariate normal random vector satisfying $EX_i = 0$, $EX_i^2 = 1$ and $EX_i X_j = r(i, j)$ for $i, j = 1, 2, \dots, p$. Let H_m denote the Hermite polynomial of order m , with leading coefficient equal to 1. For example $H_0(x) = 1$, $H_1(x) = x$, $H_2(x) = x^2 - 1$, $H_3(x) = x^3 - 3x$, \dots , (see [1, p. 133]). Then the moment $E H_m(X_1) H_m(X_2) \cdots H_m(X_p)$ is again given by (2.1) but with $K = 1$ and with $R(i_1, j_1, i_2, j_2, \dots, i_q, j_q)$ equal to the product $r(i_1, j_1) r(i_2, j_2) \cdots r(i_q, j_q)$.

(5) Set $X_1 = X_2 = \cdots = X_p$ in the preceding remark. Then $r(i, j) = 1$ for all $i, j = 1, 2, \dots, p$. Using (2.1) we obtain the following counting formula:

$$\frac{(m!)^p}{2^{mp/2} (\frac{1}{2}mp)!} \sum 1 = E(H_m(X))^p \quad (2.3)$$

where \sum is defined as in (2.1) and where X denotes a $N(0, 1)$ random variable.

The values of the normalized moments,

$$\frac{E(H_m(X))^p}{(E(H_m(X))^2)^{p/2}} = E\left(\frac{H_m(X)}{(m!)^{1/2}}\right)^p = \frac{(m!)^{p/2}}{2^{mp/2} (\frac{1}{2}mp)!} \sum 1,$$

can be found in the last column of Table 4. These values are of interest because the random variable $\bar{Z}_m(1)$, with a parameter H equal to 1, can be defined as $(m!)^{-1/2} H_m(X)$. The following remark elaborates on this point.

(6) Taqqu [12] and Dobrushin and Major [3] have shown that

$$\frac{1}{d_N} \sum_{i=1}^{[Nr]} H_m(X_i) \Rightarrow \bar{Z}_m(t) \quad (2.4)$$

as $N \rightarrow \infty$ when the X_i form a stationary normalized Gaussian sequence with covariance $r(i, j) \sim |i - j|^{-D}$ as $|i - j| \rightarrow \infty$ and when $d_N^2 = \text{var}(\sum_{i=1}^N H_m(X_i))$. The symbol ' \Rightarrow ' means here convergence of the finite-dimensional distributions. As $N \rightarrow \infty$, one has $1/d_N \sim K/N^H$ where K is the constant defined in (2.1) and where $H = 1 - \frac{1}{2}mD \in (\frac{1}{2}, 1)$ is the self-similarity parameter of $\bar{Z}_m(t)$.

Now, consider the case of perfect dependence $X = X_1 = X_2 = \cdots$. One can think of this case as corresponding to $H = 1$ because, when $H = 1$, one has $1/d_N \sim K/N$ with $K = (m!)^{-1/2} = (E(H_m(X))^2)^{-1/2}$; and, with such a d_N ,

$$\frac{1}{d_N} \sum_{i=1}^{[Nr]} H_m(X) \Rightarrow \frac{H_m(X)}{(m!)^{1/2}} t$$

as $N \rightarrow \infty$. The limiting process is self-similar with a self-similarity parameter $H = 1$.

The analogy with (2.4) suggests the definition

$$\bar{Z}_m(t) = \frac{H_m(X)}{(m!)^{1/2}} t$$

when $H = 1$.

3. Multigraph formulation

The specification of all sequences $(i_1, j_1, \dots, i_q, j_q)$ on which the summation \sum is to be performed can be efficiently systematized through the introduction of *multigraphs*.

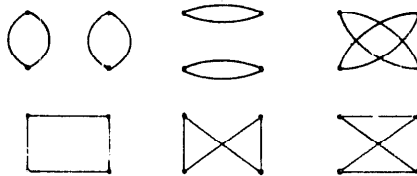
A multigraph is defined as in Harary [5]. It has multiple edges but no loops. We suppose that its vertices are labelled but not its edges. Let A denote such a multigraph. The p vertices of A are labelled $1, \dots, p$ and its q edges are denoted $(i_1, j_1), (i_2, j_2), \dots, (i_q, j_q)$. The indices $i_1, j_1, \dots, i_q, j_q$ take values in $\{1, \dots, p\}$ and each pair (i_s, j_s) , $s = 1, \dots, q$ symbolizes the existence of an edge joining the vertex i_s to the vertex j_s . Identical pairs indicate the presence of multiple edges. The absence of loops is expressed through the requirement $i_s \neq j_s$ for all $s = 1, \dots, q$.

A multigraph is *m-regular* if each vertex has degree m , that is if there are exactly m edges incident to each vertex.

Let $\mathcal{A}_p(m)$ denote the set of all multigraphs with p vertices that are m -regular. $\mathcal{A}_p(m)$ is non-empty when $p \geq 2$ with mp even, and in that case, each multigraph in $\mathcal{A}_p(m)$ has exactly $q = \frac{1}{2}mp$ lines. For instance, the three multigraphs in $\mathcal{A}_4(1)$ are



and the six multigraphs in $\mathcal{A}_4(2)$ are



With each multigraph $A \in \mathcal{A}_p(m)$ associate a *multiplicity number* $g(A)$ defined as follows. Number each of the $\binom{p}{2}$ possible pair of vertices by $u = 1, 2, \dots, \binom{p}{2}$. Let v_u be the number of edges in A joining the pair of vertices numbered u . If A has q edges, then obviously $v_1 + v_2 + \dots + v_{\binom{p}{2}} = q$. Define then

$$g(A) = \prod_{u=1}^{\binom{p}{2}} \frac{1}{v_u!}.$$

For instance,

$$g\left(\boxed{}\right) = 1$$

whereas,

$$g\left(\bigcirc \bigcirc\right) = \frac{1}{2!2!} = \frac{1}{4}.$$

Theorem 3.1 ([10, Corollary 4.1]). *The moments of $\bar{Z}_m(1)$ can be expressed as*

$$E(\bar{Z}_m(1))^p = K^p (m!)^p \sum_{A \in \mathcal{A}_p(m)} g(A) R(A) \quad (3.1)$$

where

$$\begin{aligned} R(A) &= R(i_1, j_1, i_2, j_2, \dots, i_q, j_q) \\ &= \int_0^1 \cdots \int_0^1 |x_{i_1} - x_{j_1}|^{-D} |x_{i_2} - x_{j_2}|^{-D} \cdots |x_{i_q} - x_{j_q}|^{-D} dx_1 \cdots dx_p, \end{aligned}$$

if A denotes the multigraph with lines $(i_1, j_1), (i_2, j_2), \dots, (i_q, j_q)$.

Remark 3.2. Remarks similar to those of the preceding section can be made here. In particular, one has

$$(m!)^p \sum_{A \in \mathcal{A}_p(m)} g(A) = E(H_m(X))^p. \quad (3.2)$$

4. Algorithm for generating all multigraphs in $\mathcal{A}_p(m)$

Any multigraph $A \in \mathcal{A}_p(m)$ can be characterized by the adjacency matrix $\{n_{ij}; i, j = 1, \dots, p\}$ where n_{ij} denotes the number of edges joining the vertex i to the vertex j . The relevant information about A is already contained in the upper-triangular part of the adjacency matrix because $n_{ii} = 0$ and $n_{ij} = n_{ji}$. Note also that $\sum_{j=1}^p n_{ij} = m$ since each vertex i has exactly degree m .

The set of all adjacency matrices corresponding to multigraphs in $\mathcal{A}_p(m)$ is the set of all feasible solutions to the following constraints

$$\begin{aligned} \sum_{j=1}^p n_{ij} &= m, & 0 \leq n_{ij} \leq m, \\ n_{ij} &\text{ integer,} & n_{ij} = n_{ji}, \end{aligned} \quad (i, j = 1, \dots, p). \quad (4.1)$$

This formulation leads to an implicit enumeration algorithm.

The idea behind the algorithm is as follows. One starts by fixing the first line of the adjacency matrix in such a way that the elements n_{ij} , $j = 1, \dots, p$ sum up to m . This defines the edges incident to the first vertex of the multigraph. Then one

turns to the second line of the adjacency matrix and completes all assignments of integers to the second of the upper-triangular part of the matrix, consistent with the requirement that the sum of all elements of the second line equals m . Then one turns to the third line of the adjacency matrix, etc.

It is convenient to formulate the algorithm in terms of an *enumeration tree*. Each level of the tree corresponds to a vertex and thus, to the position of a line of the adjacency matrix.

At the first level of the tree, one starts by considering all possible solutions of $\{\sum_{j=1}^p n_{1j} = m, n_{1j} \geq 0 \text{ integer}\}$. Choosing a specific solution specifies the first line of the matrix and thus all edges incident to the corresponding vertex in a given multigraph $A \in \mathcal{A}_p(m)$.

When reaching the level i_0 ($1 \leq i_0 \leq p-1$) of the matrix, all the elements

$$\{n_{ij}, (i < i_0, j = 1, \dots, p) \cup (j < i_0, i = 1, \dots, p)\}$$

have already been characterized. One looks then at all possible assignments of non-negative integers n_{i_0j} , $j > i_0$ consistent with the requirement $\sum_{j=1}^p n_{i_0j} = m$. Naturally, this takes into account the numbers assigned at the previous levels. A specific solution at level i_0 , where $1 \leq i_0 \leq p-1$, is thus a vector

$$(n_{i_0, i_0+1}, n_{i_0, i_0+2}, \dots, n_{i_0, p})$$

characterizing the edges incident to the vertex i_0 .

If no such vector can be found (infeasibility), the algorithm goes back to the previous level (goes backward up the tree) and tries another solution for the level $i_0 - 1$.

After $p-1$ solutions have been chosen, one for each of the $p-1$ levels, feasibility can again be checked by summing the p th row of the adjacency matrix. If the sum equals m , the completed matrix represents an m -regular multigraph.

Upon completing a matrix, the algorithm systematically goes back to an earlier level i_0 , $i \leq i_0 \leq p-1$, chooses a new solution for the level i_0 , and thus starts following another branch of the enumeration tree. Eventually, all possible solutions are evaluated and all multigraphs in $\mathcal{A}_p(m)$ are characterized.

The number of multigraphs in $\mathcal{A}_p(m)$ for $p = 1, \dots, 6$ and $m = 1, \dots, 9$ is given in Table 1.

5. Equivalence classes

Different $A \in \mathcal{A}_p(m)$ may yield the same value of $R(A)$ and therefore the amount of computation can be significantly decreased by partitioning $\mathcal{A}_p(m)$ into equivalence classes.

Definition 5.1. Two multigraphs A and A' are *isomorphic* if there exists a permutation π of the vertices of A which satisfies the following condition: if there are n

Table 1^a. Number of multigraphs in $\mathcal{A}_p(m)$ for various values of m and p .

| $p \backslash m$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|----|-----|-----|------|----|----|----|----|----|
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3 | 0 | 1 | 0 | 1 | 0 | 1 | 0 | 1 | 0 |
| 4 | 3 | 6 | 10 | 15 | 21 | 28 | 36 | 45 | 55 |
| 5 | 0 | 22 | 0 | 158 | 0 | — | 0 | — | 0 |
| 6 | 15 | 130 | 760 | 3355 | — | — | — | — | — |

^a The number is 0 when mp is odd. Cases marked with a bar were not computed due to excessive computer time. For instance, the determination and printout of all the multigraphs in $\mathcal{A}_p(m)$ for $m=4$ and for $p=2, \dots, 6$ took 12 minutes using the PL/C computing language on an IBM 370. PL/C is a diagnostic language which is significantly slower than PL/I.

edges between the vertices i and j of A , then and only then will there be n edges between the vertices πi and πj of A' .

Example 5.2. The multigraphs



are isomorphic.

Proposition 5.3. $R(A)$, $A \in \mathcal{A}_p(m)$ is invariant under isomorphism.

Proof. A permutation of the vertices of A corresponds to a permutation in the variables in the integral expressing $R(A)$. Such a permutation obviously preserves the value of the integral.

Remark 5.4. The proposition does not hold if $R(A)$ is replaced by the expression

$$R_{(i_1, \dots, i_p)}(A) = R_{(i_1, \dots, i_p)}(i_1, j_1, \dots, i_q, j_q)$$

of (2.2).

If one could determine all multigraphs that are isomorphic to a given multigraph A , then it would only be necessary to evaluate a single integral $R(A)$ for each equivalence class.

Unfortunately, it is not known whether there exists an algorithm for characterizing these equivalence classes in polynomial time [4, p. 285]. An alternative is to broaden the equivalence classes. One way to proceed is as follows.

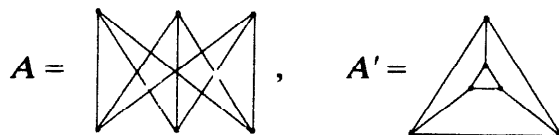
Recall that to each multigraph $A \in \mathcal{A}_p(m)$, one can associate an upper-triangular matrix with elements n_{ij} , $i < j$, $i, j = 1, \dots, p$, where n_{ij} denotes the number of edges

connecting the vertices i and j . Let

$$\{y_u, u = 1, \dots, \binom{p}{2}\} = \{n_{ij}, i < j, i, j = 1, \dots, p\}.$$

Say that two multigraphs A and A' are *isomorphic** if their corresponding sequences $\{y_u, u = 1, \dots, \binom{p}{2}\}$ and $\{y'_u, u = 1, \dots, \binom{p}{2}\}$ differ by a permutation.

Two isomorphic multigraphs are necessarily isomorphic*. But the converse is false. Consider for example the two graphs



which belong to $\mathcal{A}_6(3)$. They are isomorphic*, but they are not isomorphic. Indeed, A is the 'utility graph' which is known to be non-planar. A' is planar and therefore A and A' cannot be isomorphic.

To decide whether two multigraphs A and A' of $\mathcal{A}_m(p)$ are isomorphic* it is sufficient to compare the corresponding sequences $(y_u, u = 1, \dots, \binom{p}{2})$ and $(y'_u, u = 1, \dots, \binom{p}{2})$. Each sequence has $\binom{p}{2}$ entries and each entry is at most equal to m . The entries of a sequence can be ordered in $O(\binom{p}{2})$ steps by recording the number of entries that are respectively equal to $0, 1, \dots, m$ (the 'bucket sort method'). Isomorphism* can thus be detected in polynomial time.

Isomorphism* is a useful notion because

(i) for small p and m , isomorphic* multigraphs are isomorphic (see Fig. 1 for example),

(ii) as a first approximation, one can set $R(A) \cong R(A')$ for isomorphic* multigraphs A and A' (This approximation is only used here for the cases $p = 4, m = 5$ and $p = 6, m = 3$).

In some applications, a better approximation may be required. One can then define the notion of isomorphism** by requiring that two isomorphism** multigraphs be isomorphic* and in addition, share some additional common characteristics.

Table 2 gives the number of isomorphic and isomorphic* equivalence classes and Fig. 1 lists a representative of each of these classes. These tables can be conveniently referred to when computing the moments of some other non-linear function of a Gaussian variable.

6. Evaluation of the integrals

We must compute

$$R(A) = \int_0^1 \cdots \int_0^1 g_A(x_1, \dots, x_p) dx_1 \cdots dx_p$$

(a)

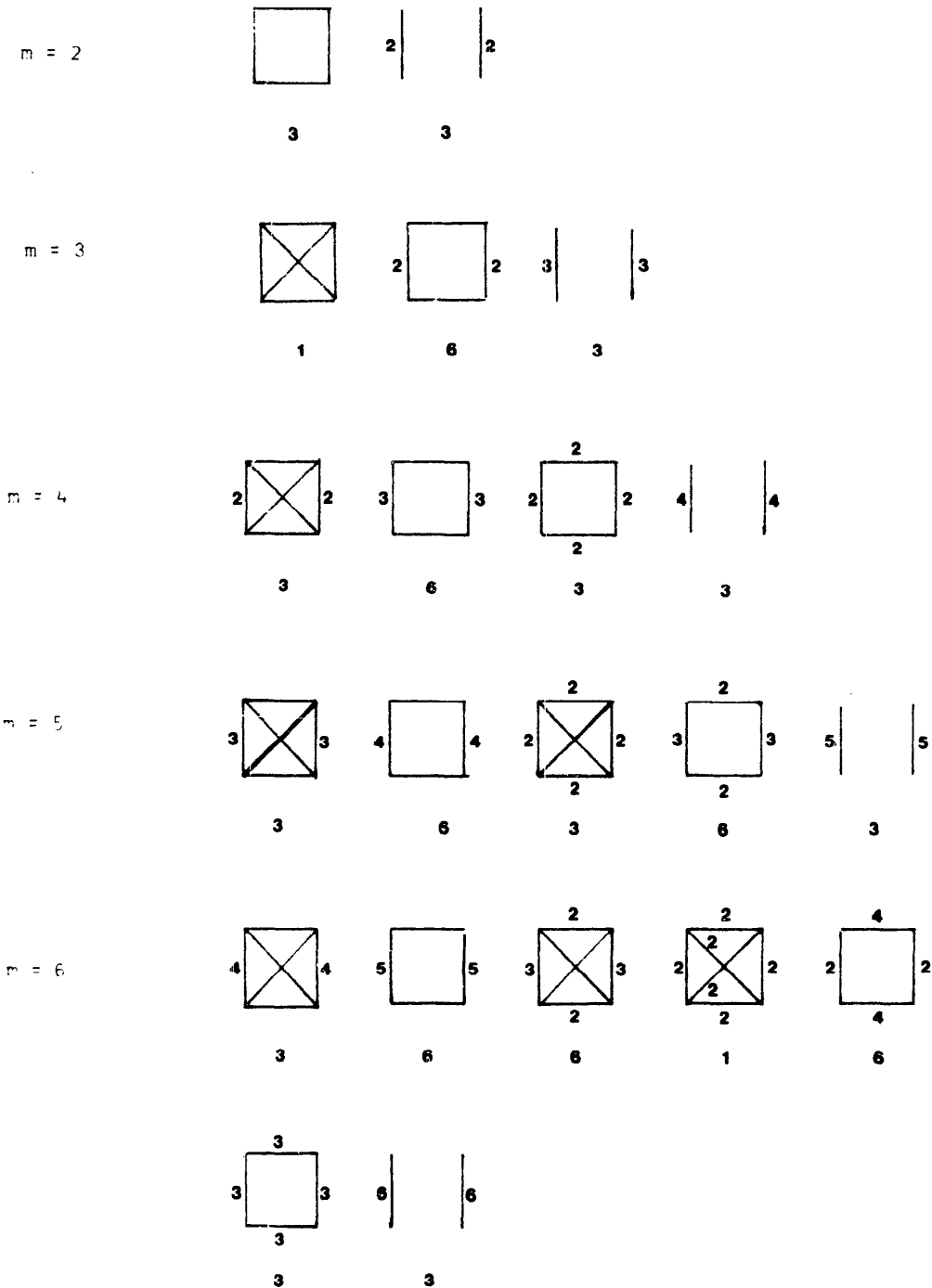


Fig. 1. Exhaustive list of representative multigraphs for each equivalence class in $\mathcal{A}_p(m)$. (a) $m = 2, \dots, 9, p = 4$; (b) $m = 2, p = 3, 5, 6$; (c) $m = 3, p = 6$; (d) $m = 4, p = 5$.

For convenience the multiplicity of the edges is indicated by a number placed on the edge. Multigraphs corresponding to $m = 2, \dots, 9, p = 4$ (Fig. 1(a)) and $m = 2, p = 3, 5, 6$ (Fig. 1(b)) are representative of isomorphic equivalence classes. The multigraphs for $m = 3, p = 6$ (Fig. 1(c)) and $m = 4, p = 5$ (Fig. 1(d)) are representative of isomorphic* equivalence classes. The number below a representative multigraph indicates the size of the corresponding equivalence class.

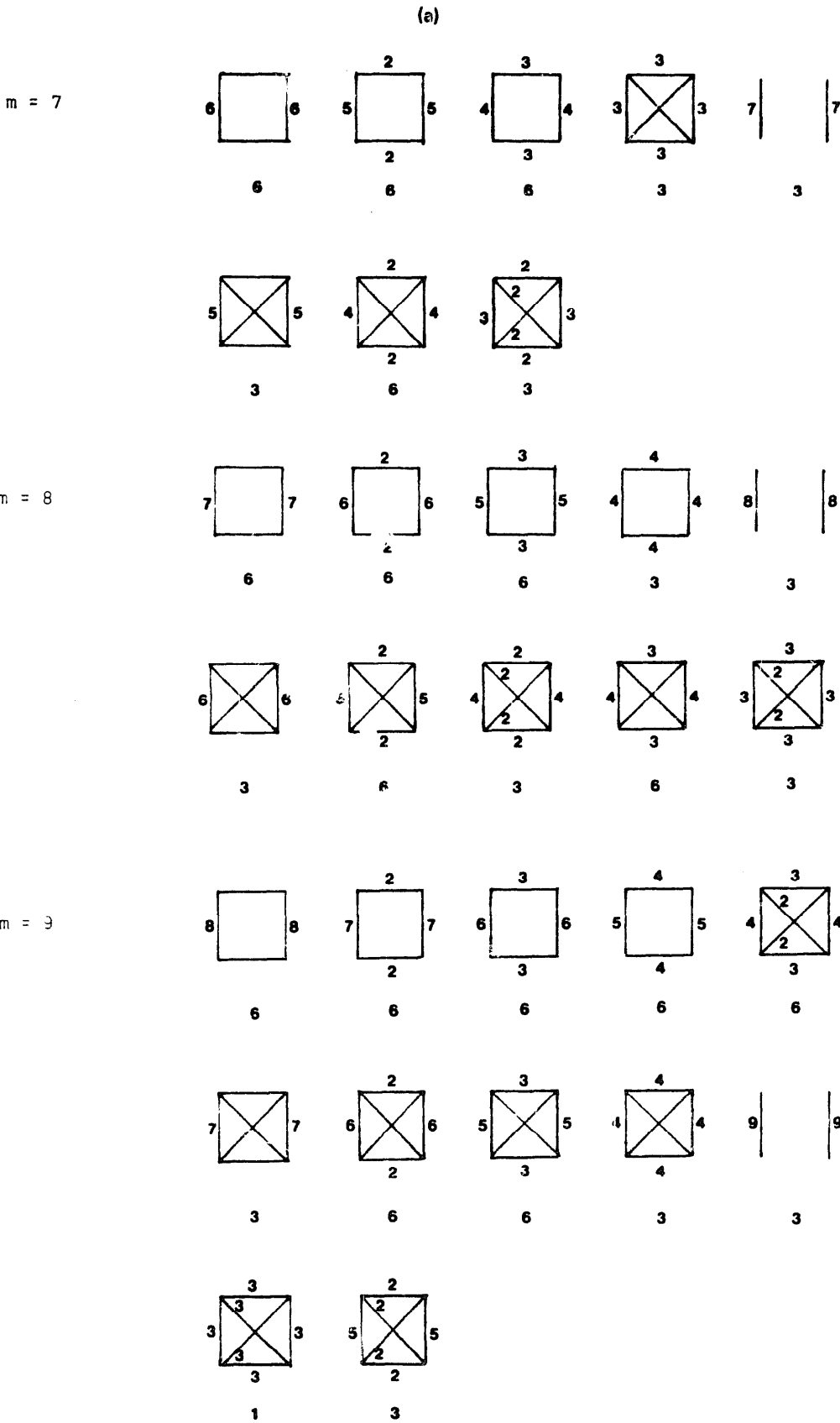


Fig. 1 (cont.)

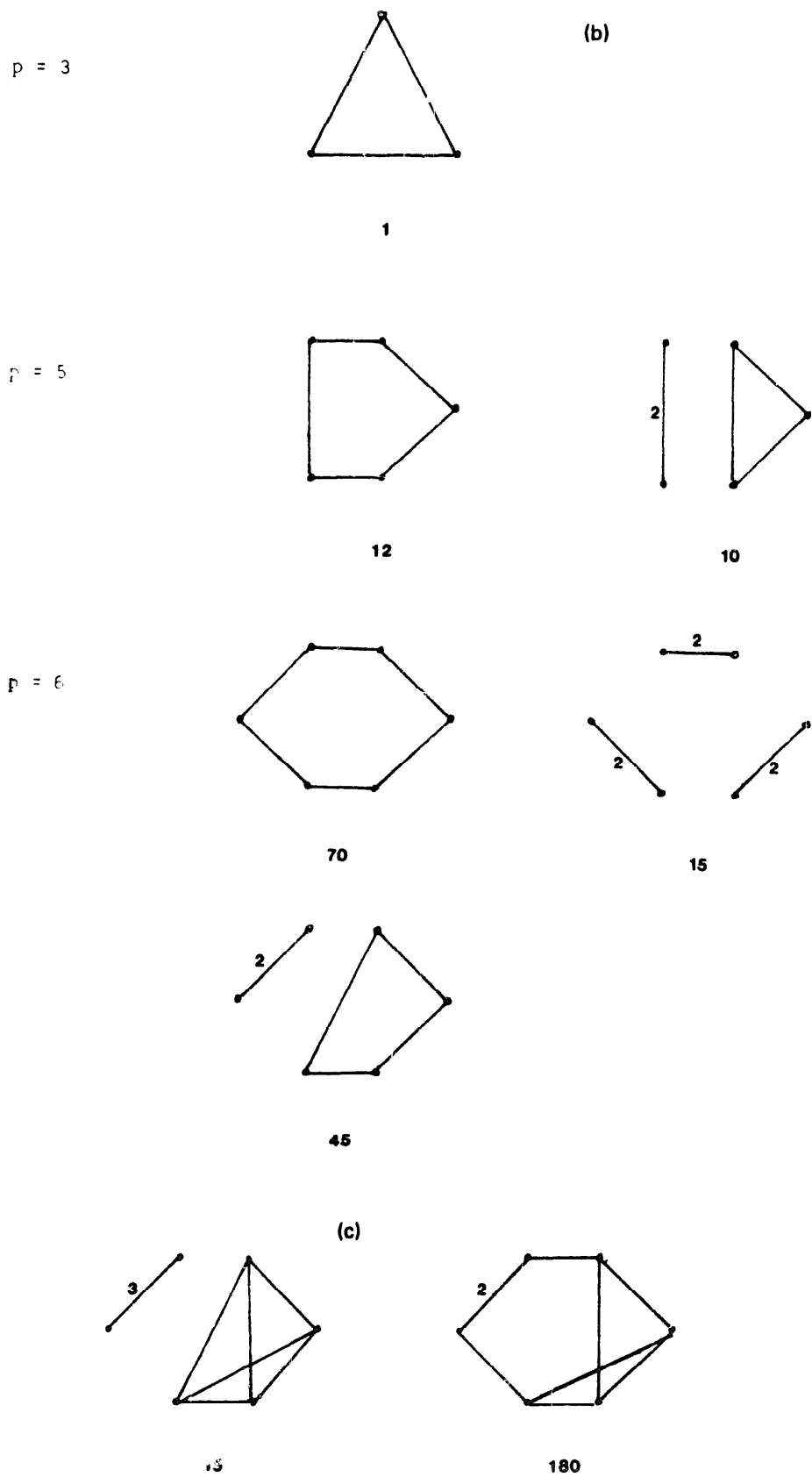


Fig. 1 (cont.)

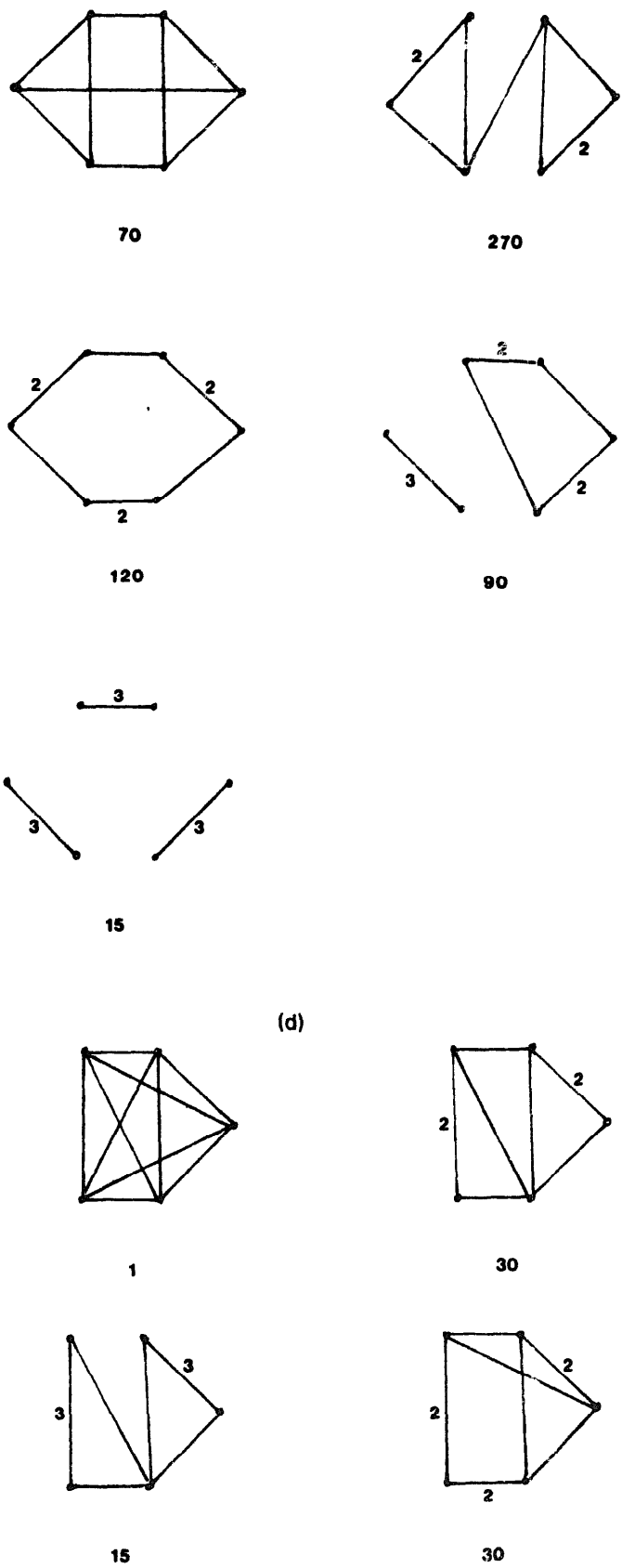


Fig. 1 (cont.)

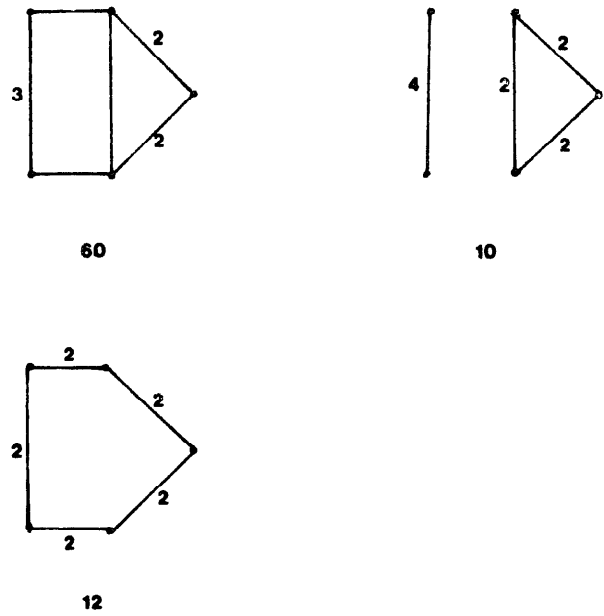


Fig. 1 (cont.)

Table 2. Number of isomorphic and isomorphic* equivalence classes of multigraphs in $\mathcal{A}_p(m)$.

| $p \backslash m$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|------------------|---|---|-----------------|-----------------|---|---|---|----|----|
| 2 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 3 | 0 | 1 | 0 | 1 | 0 | 1 | 0 | 1 | 0 |
| 4 | 1 | 2 | 3 | 4 | 5 | 7 | 8 | 10 | 12 |
| 5 | 0 | 2 | 0 | 7* ^a | 0 | — | 0 | — | 0 |
| 6 | 1 | 3 | 7* ^a | — | — | — | — | — | — |

^a A star refers to the number of isomorphic* equivalence classes.

where

$$g_A(x_1, \dots, x_p) = |x_{i_1} - x_{j_1}|^{-D} |x_{i_2} - x_{j_2}|^{-D} \dots |x_{i_q} - x_{j_q}|^{-D},$$

$A \in \mathcal{A}_p(m)$, $0 < D < 1/m$, $q = \frac{1}{2}mp$, and where $(i_1, j_1), (i_2, j_2), \dots, (i_q, j_q)$ denote the edges of A .

When $p = 2$,

$$R(A) = \int_0^1 \int_0^1 |x_1 - x_2|^{-mD} dx_1 dx_2 = \frac{2}{(1 - mD)(2 - mD)}$$

for any $A \in \mathcal{A}_2(m)$, $m \geq 1$. But there is no formula known for evaluating $R(A)$ for arbitrary $A \in \mathcal{A}_p(m)$.

We evaluate the integrals $R(A)$ numerically when $p \geq 3$.

Because of the divergence of the integrand $g_A(x_1, \dots, x_p)$, a linear approximation of the type

$$\frac{1}{N^p} \sum_{x_1=1}^N \cdots \sum_{x_p=1}^N g_A(x_1, \dots, x_p)$$

is slow and imprecise. A logarithmic scale around the hyper-diagonals would improve the approximation but is difficult to implement when p is large.

A Monte Carlo simulation was the most successful method attempted. N independent random vectors (X_1, \dots, X_p) , each vector consisting of p independent and identically distributed uniform random variables on $(0, 1)$ were generated. Then the following quantity

$$R_N(A) = \frac{1}{N} \sum_{k=1}^N (g_A(X_1, \dots, X_p))_k$$

was evaluated. The strong law of large numbers ensures that $R_N(A)$ converges to $R(A)$ almost everywhere as N tends to infinity.

This method applied to the single integral $\int_0^1 x^{-0.25} dx = 1.3333$ yielded a value of 1.3324 with $N = 30000$. When applied to the double integral $\int_0^1 \int_0^1 |x - y|^{-0.25} dx dy = 1.5238$, it yielded 1.5184 with $N = 30000$. Higher values of N (up to 10^6) did not improve the numerical results significantly.

The Monte Carlo evaluation of $R(A)$ constituted a subset of the program evaluating the moments of $\bar{Z}_m(1)$. However, when $m = 2$, the $R(A)$'s involving connected multigraph A 's were evaluated separately because of their special interest. The results of this evaluation are stated in the next section.

7. Numerical values of the integrals corresponding to cycle graphs

When $m = 2$, the components of the multigraphs $A \in \mathcal{A}_p(2)$ are cycle graphs. If a multigraph $A \in \mathcal{A}_p(2)$ is a cycle graph with only one component, it will have p vertices, p edges, and satisfy the relation

$$R(A) = I(p)$$

where

$$I(p) = \int_0^1 \int_0^1 \cdots \int_0^1 |x_1 - x_2|^{-D} |x_2 - x_3|^{-D} \cdots \\ \times |x_{p-1} - x_p|^{-D} |x_p - x_1|^{-D} dx_1 dx_2 \cdots dx_p.$$

The integrals $I(p)$ appear in various other contexts as well. For example, the cumulants of the normalized $\bar{Z}_2(1)$ are

$$\kappa_p = (p-1)! 2^{p-1} \frac{I(p)}{I(2)}, \quad p \geq 2.$$

Also, $I(p)$ is the trace of the p th iteration^{*} of the Hilbert–Schmidt kernel,

$$K(x, y) = |x - y|^{-D}, \quad 0 < D < \frac{1}{2}$$

on $L^2(0, 1)$. In fact, if $\lambda_j, j = 1, 2, \dots$, denote the eigenvalues of the integral equation

$$\int_0^1 |x - y|^{-D} f(y) \, dy = \lambda f(x),$$

then

$$\sum_{j=1}^\infty (\lambda_j)^p = I(p).$$

Table 3 lists the exact value of $I(2)$ and the Monte Carlo evaluations of $I(p)$ for $p = 3, 4, 5, 6$ and $D = 0.1, 0.2, 0.3, 0.4$. To illustrate the reliability of the Monte Carlo evaluations, we list here the values of an estimate of the standard deviation. That estimate was defined as $s^2(p) = \sum_{i=1}^{30} (Y_i - \hat{I}(p))^2 / 29$, where each Y_1, Y_2, \dots, Y_{30} is an average of 1000 independent evaluations of $I(p)$, and where $\hat{I}(p) = \sum_{i=1}^{30} Y_i / 30$. Then, for $D = 0.3$: $\hat{I}(3) = 4.943, s^2(3) = 0.044$; $\hat{I}(4) = 8.137, s^2(4) = 0.080$; $\hat{I}(5) = 13.462, s^2(5) = 0.351$; $\hat{I}(6) = 22.714, s^2(6) = 1.067$. When $D = 0.2$, $\hat{I}(4) = 3.738, s^2(4) = 0.0064$.

Table 3. Numerical values of $I(p)$, the integrals corresponding to cycle graphs. These cycle graphs are components of the multigraphs in $\mathcal{A}_p(2)$.

| | $D = 0.1$ | $D = 0.2$ | $D = 0.3$ | $D = 0.4$ |
|--------|-----------|-----------|-----------|-----------|
| $I(2)$ | 1.4 | 2.1 | 3.6 | 8.3 |
| $I(3)$ | 1.6 | 2.7 | 4.9 | 10.3 |
| $I(4)$ | 1.9 | 3.7 | 8.1 | 19.4 |
| $I(5)$ | 2.2 | 5.2 | 13.5 | 39.5 |
| $I(6)$ | 2.6 | 7.2 | 22.7 | 82.8 |

8. Numerical values of the moments of $\tilde{Z}_m(1)$

Table 4 lists the numerical values of the moments $E(\tilde{Z}_m(1))^p$ for $m = 2, 3, \dots, 8$ and $p = 3$ up to 6, when $H = 0.6, 0.7, 0.8, 0.9$. These values are obtained by combining the results of the preceding sections and applying (3.1). Recall that $E(\tilde{Z}_m(1))^2 = 1$ and $E(\tilde{Z}_m(1))^p = 0$ for mp odd.

The numerical values have been rounded. The lowest digit is uncertain but the preceding one is usually significant. The higher the value of H , the more precise is the evaluation. The last column of Table 4 gives the moments of the random variable $(m!)^{-1/2} H_m(X)$. As indicated in Section 2, that random variable refers to

Table 4. Monte Carlo evaluations of $E(\bar{Z}_m(1))^p$ for various values of m , p and of the self-similarity parameter H .

| | $H = 0.6$ | $H = 0.7$ | $H = 0.8$ | $H = 0.9$ | Theoretical upper bound ($H = 1$) |
|---------|-----------|-----------|-----------|-----------|-------------------------------------|
| $m = 2$ | | | | | |
| $p = 3$ | 1.2 | 2.06 | 2.55 | 2.77 | 2.83 |
| $p = 4$ | 6. | 11. | 13.3 | 14.7 | 15.00 |
| $p = 5$ | 26. | 60. | 81.8 | 93.2 | 96.17 |
| $p = 6$ | 148. | 425. | 620. | 726. | 755.60 |
| $m = 3$ | | | | | |
| $p = 4$ | 29. | 61. | 81. | 90.5 | 93.00 |
| $m = 4$ | | | | | |
| $p = 3$ | 6. | 11. | 13.3 | 14.4 | 14.70 |
| $p = 4$ | 180. | 403. | 550.0 | 620. | 639.00 |
| $m = 5$ | | | | | |
| $p = 4$ | 1300. | 2890. | 3970. | 4507. | 4653.00 |
| $m = 6$ | | | | | |
| $p = 3$ | 37. | 65. | 80.5 | 87.5 | 89.44 |
| $m = 8$ | | | | | |
| $p = 3$ | 240. | 420. | 524. | 572. | 585.60 |

the case of perfect correlation and therefore corresponds to the limiting value ' $H = 1$ '.

We note that the moments increase with m . This is consistent with the following corollary of a result of McKean [8]: there exist non-negative constants C_* , a_* , C^* , a^* such that

$$C_* e^{-a_* x^{2/m}} \leq \mathbf{P}\{\bar{Z}_m(1) > x\} \leq C^* e^{-a^* x^{2/m}}$$

for $x > 0$.

The computed moments of $\bar{Z}_m(1)$ also increase with H , suggesting that the distribution tails $\mathbf{P}\{\bar{Z}_m(1) > |x|\}$, $|x|$ large, may increase with H as well.

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